CALIFORNIA INSTITUTE OF TECHNOLOGY

BECKMAN INSTITUTE

X-RAY CRYSTALLOGRAPHY LABORATORY

Date 6 August 2010

Crystal Structure Analysis of:

MSW03

(shown below)

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Advisor: J. E. Bercaw. ext. 6577

Account Number: JEB.65152-1-DOE.651520

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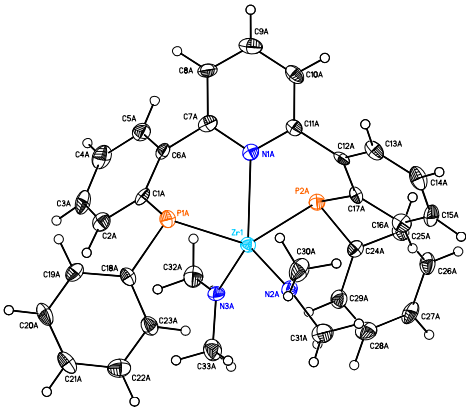
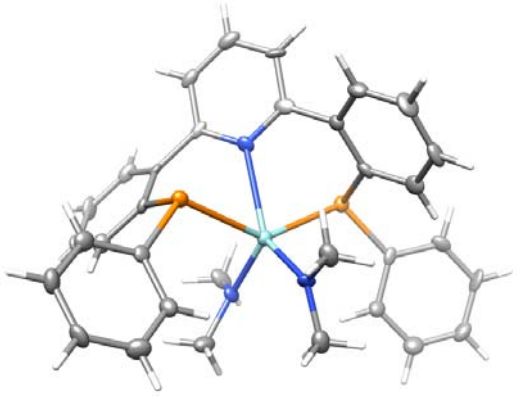
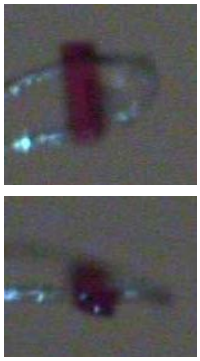




MSW03

Note: The crystallographic data have been deposited in the Cambridge Database (CCDC) and has been placed on hold pending further instructions from me. The deposition number is 787542. Ideally the CCDC would like the publication to contain a footnote of the type: "Crystallographic data have been deposited at the CCDC, 12 Union Road, Cambridge CB2 1EZ, UK and copies can be obtained on request, free of charge, by quoting the publication citation and the deposition number 787542."

Table 1. Crystal data and structure refinement for MSW03 (CCDC 787542).



Empirical formula	$C_{33}H_{33}N_3P_2Zr \bullet ¼ (C_6H_6)$
Formula weight	644.31
Crystallization Solvent	Benzene/pentane
Crystal Habit	Blade
Crystal size	0.22 x 0.07 x 0.01 mm^3
Crystal color	Orange/red

Data Collection

Type of diffractometer	Bruker KAPPA APEX II	
Wavelength	0.71073 Å MoKα	
Data Collection Temperature	100(2) K	
θ range for 9165 reflections used in lattice determination	2.45 to 24.48°	
Unit cell dimensions	a = 8.1980(9) Å b = 33.236(4) Å c = 23.311(2) Å	α= 90° β= 96.280(6)° γ = 90°
Volume	6313.4(12) $Å^3$	
Z	8	
Crystal system	Monoclinic	
Space group	P $2_1/c$	
Density (calculated)	1.356 Mg/m^3	
F(000)	2660	
θ range for data collection	1.23 to 25.35°	
Completeness to θ = 25.35°	89.0 %	
Index ranges	$-9 \le h \le 9$, $-39 \le k \le 38$, $-24 \le l \le 25$	
Data collection scan type	ω scans; 7 settings	
Reflections collected	51705	
Independent reflections	10283 [R_{int}= 0.0608]	
Absorption coefficient	0.477 mm^{-1}	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7452 and 0.6212	

Table 1 (cont.)

Structure solution and Refinement

Structure solution program	SHELXS-97 (Sheldrick, 2008)
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Geometric positions
Structure refinement program	SHELXL-97 (Sheldrick, 2008)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	10283 / 0 / 723
Treatment of hydrogen atoms	Riding
Goodness-of-fit on F^2	2.255
Final R indices [$I>2\sigma(I)$, 7388 reflections]	R1 = 0.0505, *w*R2 = 0.0734
R indices (all data)	R1 = 0.0852, *w*R2 = 0.0750
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.014
Average shift/error	0.000
Largest diff. peak and hole	1.692 and -0.913 e.Å^{-3}

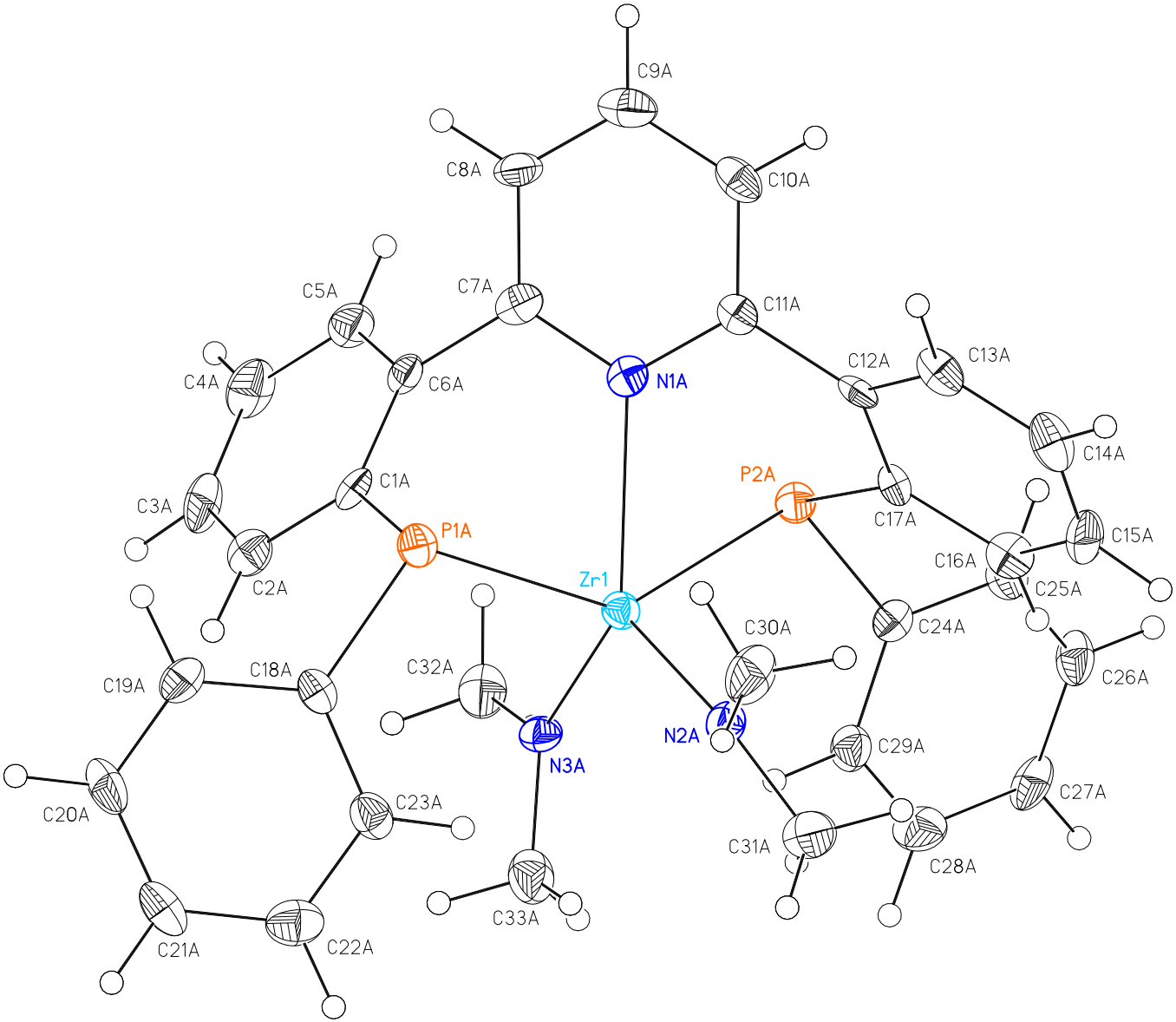
Special Refinement Details

Crystals were mounted on a loop using Paratone oil then placed on the diffractometer under a nitrogen stream at 100K.

The crystal contains solvent of crystallization. This solvent appears as rings stacked edge on along the *a*-axis and through 0, ½ , ½. The solvent was modeled as benzenes (isotropic and constrained to ideal hexagons) stacked edge to edge between the inversion centers, requiring half occupancy.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.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P2A
C17A
C3A
P1A
C15A
C16A
C2A
Zr1
C25A
C30A
C24A
C32A
C18A
C19A
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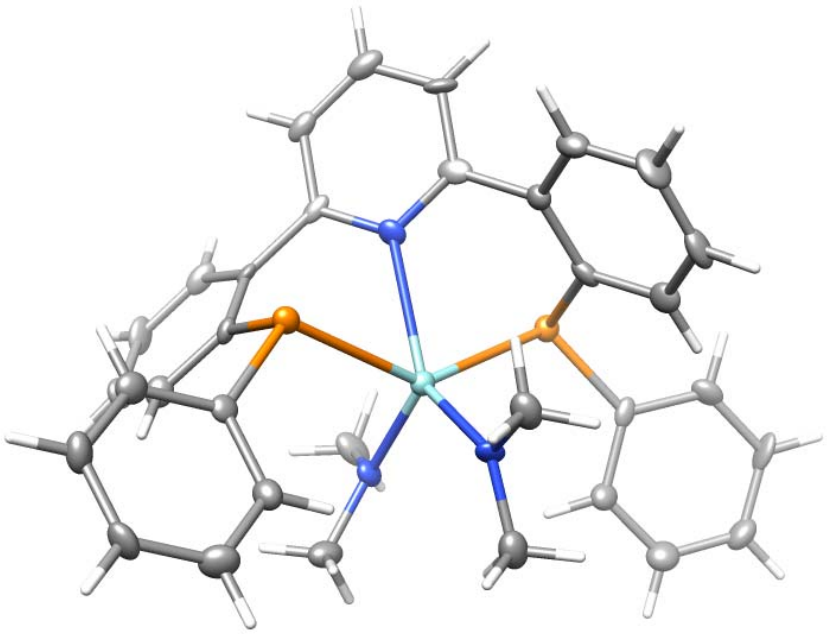

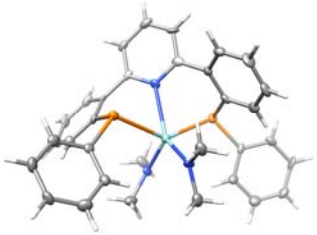

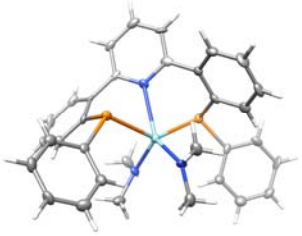

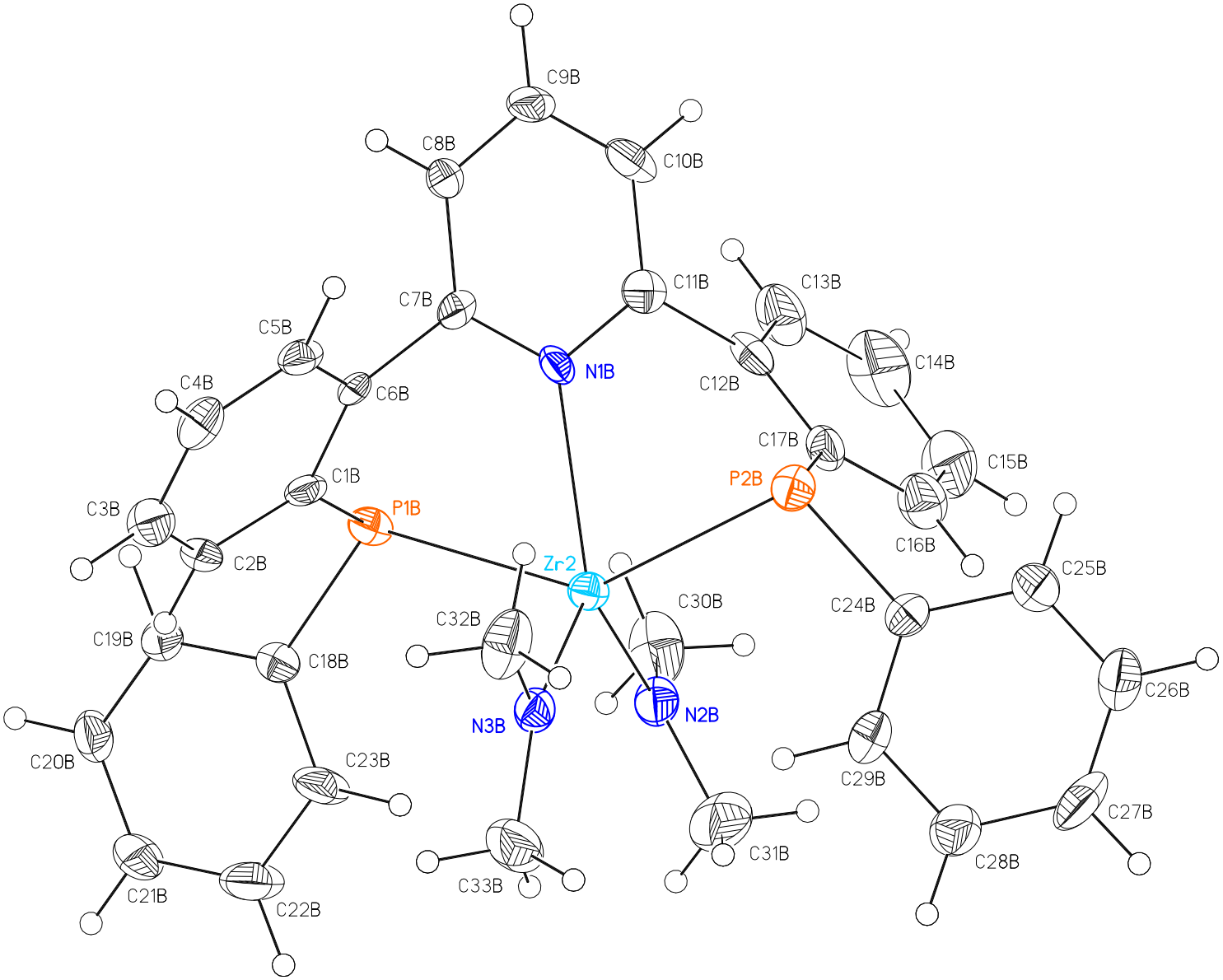
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C24B
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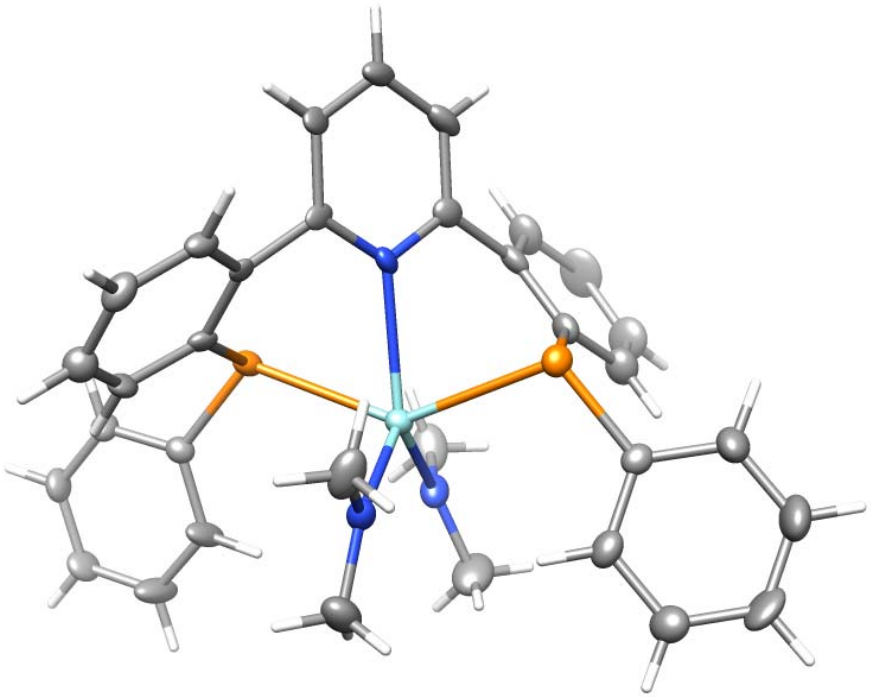

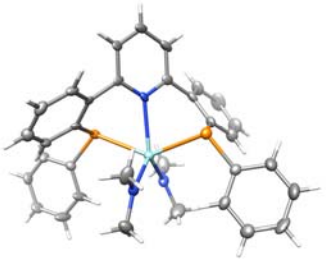

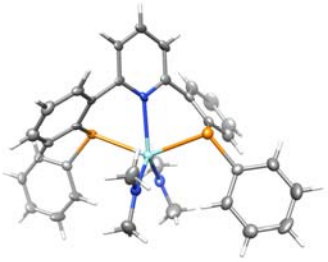

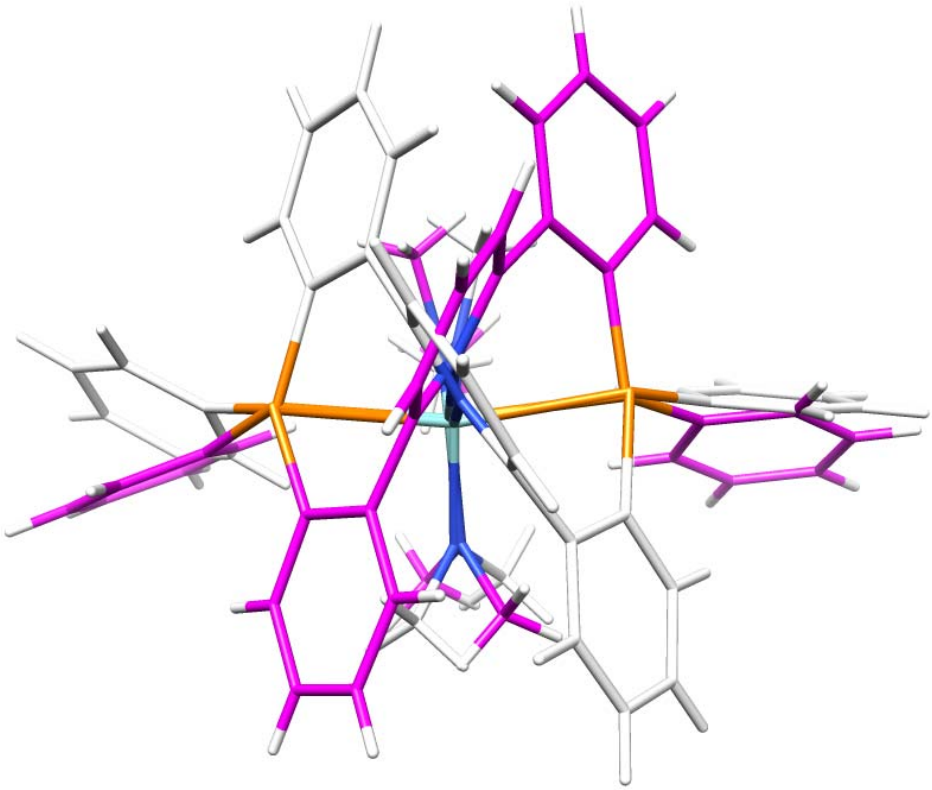

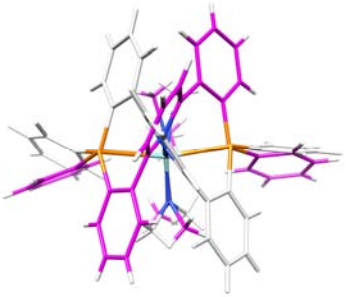

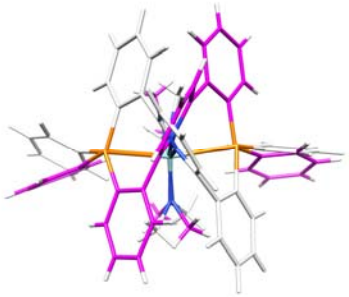

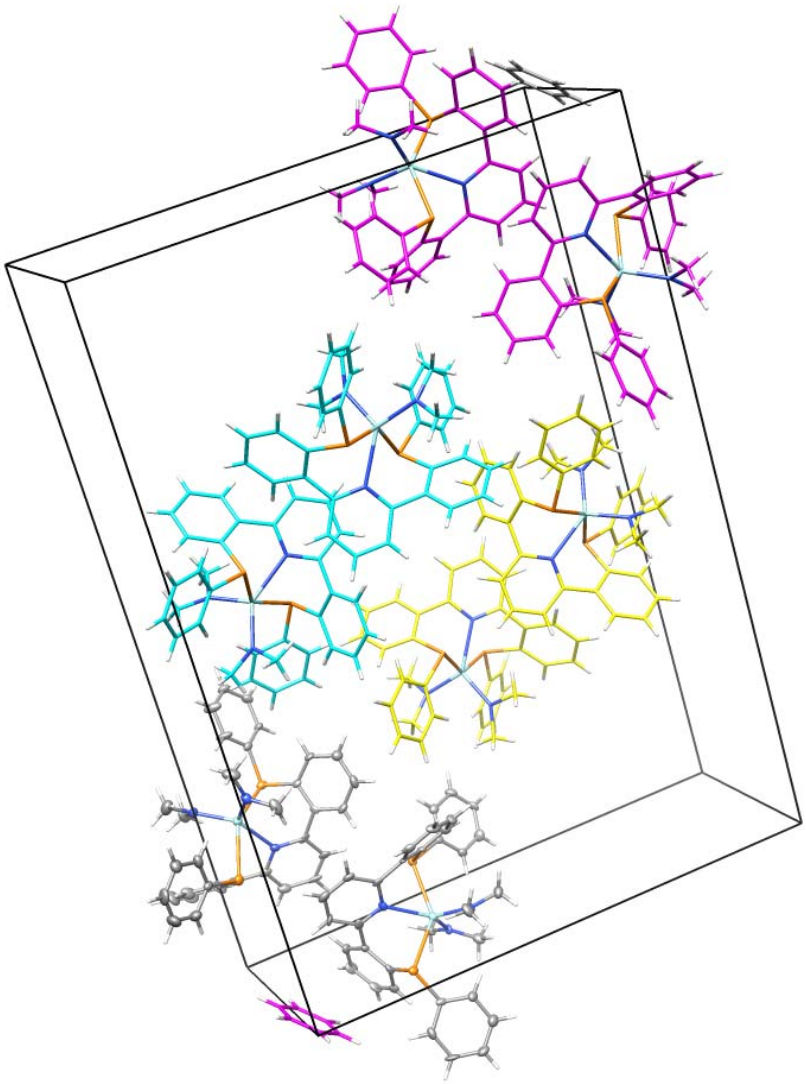

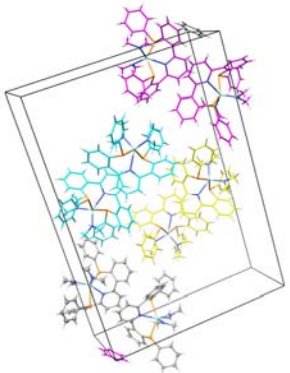

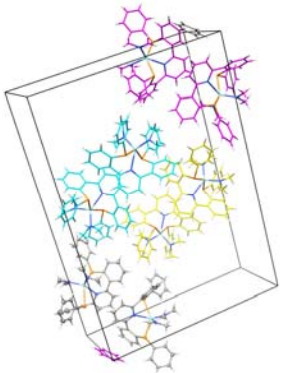

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for MSW03 (CCDC 787542). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}	Occ
Zr(1)	5078(1)	257(1)	6790(1)	16(1)	1
P(1A)	6952(1)	-110(1)	7660(1)	18(1)	1
P(2A)	2802(1)	837(1)	6595(1)	17(1)	1
N(1A)	4978(4)	672(1)	7631(2)	16(1)	1
N(2A)	6733(4)	375(1)	6248(1)	19(1)	1
N(3A)	3706(4)	-192(1)	6419(1)	18(1)	1
C(1A)	4910(5)	-226(2)	7865(2)	17(1)	1
C(2A)	4184(5)	-619(2)	7823(2)	22(1)	1
C(3A)	2668(6)	-691(2)	8002(2)	25(1)	1
C(4A)	1819(6)	-393(2)	8246(2)	29(1)	1
C(5A)	2472(6)	-11(2)	8289(2)	24(1)	1
C(6A)	3979(5)	81(1)	8096(2)	16(1)	1
C(7A)	4531(5)	506(2)	8123(2)	19(1)	1
C(8A)	4513(5)	732(2)	8622(2)	22(1)	1
C(9A)	4941(6)	1129(2)	8620(2)	27(1)	1
C(10A)	5372(5)	1302(1)	8122(2)	21(1)	1
C(11A)	5356(5)	1069(1)	7625(2)	15(1)	1
C(12A)	5647(5)	1254(1)	7072(2)	15(1)	1
C(13A)	6916(5)	1530(1)	7048(2)	21(1)	1
C(14A)	7273(6)	1704(1)	6549(2)	26(1)	1
C(15A)	6306(6)	1605(1)	6044(2)	25(1)	1
C(16A)	5001(5)	1350(1)	6054(2)	21(1)	1
C(17A)	4595(5)	1164(1)	6560(2)	15(1)	1
C(18A)	7651(5)	-601(1)	7415(2)	17(1)	1
C(19A)	7997(5)	-921(2)	7806(2)	22(1)	1
C(20A)	8609(6)	-1281(2)	7641(2)	27(1)	1
C(21A)	8935(5)	-1337(2)	7079(2)	28(1)	1
C(22A)	8623(6)	-1030(2)	6688(2)	30(1)	1
C(23A)	7996(5)	-665(1)	6851(2)	22(1)	1
C(24A)	1791(5)	862(1)	5847(2)	16(1)	1
C(25A)	908(5)	1209(1)	5669(2)	22(1)	1
C(26A)	-4(5)	1225(2)	5135(2)	24(1)	1
C(27A)	-67(6)	899(2)	4773(2)	25(1)	1
C(28A)	780(5)	553(2)	4936(2)	26(1)	1
C(29A)	1725(5)	535(1)	5472(2)	22(1)	1
C(30A)	8282(5)	558(1)	6487(2)	32(1)	1
C(31A)	6557(6)	396(1)	5621(2)	31(1)	1
C(32A)	2112(5)	-306(1)	6594(2)	27(1)	1
C(33A)	4132(6)	-449(1)	5948(2)	30(1)	1
Zr(2)	654(1)	2119(1)	9326(1)	19(1)	1
P(1B)	-1736(2)	2210(1)	8456(1)	20(1)	1
P(2B)	2698(2)	1558(1)	9831(1)	22(1)	1
N(1B)	246(4)	1505(1)	8768(2)	18(1)	1
N(2B)	-547(5)	2338(1)	9961(2)	26(1)	1
N(3B)	2276(5)	2545(1)	9177(2)	23(1)	1
C(1B)	-173(5)	2203(1)	7952(2)	18(1)	1

C(2B)	134(5)	2531(1)	7594(2)	21(1)	1
C(3B)	1275(6)	2513(2)	7199(2)	27(1)	1
C(4B)	2152(6)	2165(2)	7136(2)	28(1)	1
C(5B)	1862(5)	1837(2)	7471(2)	22(1)	1
C(6B)	739(5)	1850(1)	7877(2)	15(1)	1
C(7B)	410(5)	1481(1)	8200(2)	18(1)	1
C(8B)	168(5)	1116(2)	7906(2)	23(1)	1
C(9B)	-330(6)	784(2)	8183(2)	29(1)	1
C(10B)	-541(5)	810(2)	8757(2)	28(1)	1
C(11B)	-216(5)	1173(2)	9049(2)	22(1)	1
C(12B)	-434(6)	1206(1)	9671(2)	23(1)	1
C(13B)	-1857(6)	1046(2)	9854(2)	37(2)	1
C(14B)	-2157(7)	1067(2)	10421(3)	49(2)	1
C(15B)	-1014(7)	1257(2)	10819(2)	45(2)	1
C(16B)	415(6)	1408(2)	10641(2)	32(1)	1
C(17B)	783(6)	1387(1)	10072(2)	23(1)	1
C(18B)	-2564(5)	2723(1)	8400(2)	20(1)	1
C(19B)	-3826(5)	2806(1)	7961(2)	24(1)	1
C(20B)	-4633(6)	3172(2)	7928(2)	28(1)	1
C(21B)	-4219(6)	3463(2)	8329(2)	30(1)	1
C(22B)	-3002(6)	3388(2)	8766(2)	46(2)	1
C(23B)	-2180(6)	3023(1)	8803(2)	35(2)	1
C(24B)	3766(5)	1777(2)	10491(2)	21(1)	1
C(25B)	4428(6)	1529(2)	10940(2)	36(2)	1
C(26B)	5358(7)	1687(2)	11410(2)	49(2)	1
C(27B)	5682(6)	2093(2)	11451(2)	42(2)	1
C(28B)	5015(6)	2342(2)	11020(2)	34(1)	1
C(29B)	4069(5)	2182(2)	10543(2)	28(1)	1
C(30B)	-2188(6)	2177(2)	10009(2)	45(2)	1
C(31B)	-57(6)	2603(2)	10442(2)	51(2)	1
C(32B)	3461(6)	2399(2)	8810(2)	40(2)	1
C(33B)	2564(6)	2965(1)	9335(2)	45(2)	1
C(1C)	989(7)	10115(3)	135(3)	74(4)	0.50
C(2C)	1768(11)	9884(3)	-251(4)	308(15)	0.50
C(3C)	3469(12)	9888(3)	-228(4)	299(15)	0.50
C(4C)	4392(7)	10122(3)	181(4)	76(4)	0.50
C(5C)	3613(7)	10353(2)	567(3)	36(3)	0.50
C(6C)	1912(7)	10350(2)	544(3)	23(2)	0.50

Table 3. Selected bond lengths [Å] and angles [°] for MSW03 (CCDC 787542).

Zr(1)-N(2A)	1.991(4)	N(2A)-Zr(1)-N(3A)	105.13(14)
Zr(1)-N(3A)	2.007(3)	N(2A)-Zr(1)-N(1A)	119.45(14)
Zr(1)-N(1A)	2.406(3)	N(3A)-Zr(1)-N(1A)	135.20(14)
Zr(1)-P(2A)	2.6853(13)	N(2A)-Zr(1)-P(2A)	105.13(10)
Zr(1)-P(1A)	2.7002(12)	N(3A)-Zr(1)-P(2A)	96.56(10)
		N(1A)-Zr(1)-P(2A)	69.05(8)
		N(2A)-Zr(1)-P(1A)	101.19(10)
		N(3A)-Zr(1)-P(1A)	103.47(10)
		N(1A)-Zr(1)-P(1A)	73.39(9)
		P(2A)-Zr(1)-P(1A)	141.26(4)
Zr(2)-N(3B)	1.999(4)	N(3B)-Zr(2)-N(2B)	105.09(16)
Zr(2)-N(2B)	2.004(4)	N(3B)-Zr(2)-N(1B)	123.98(15)
Zr(2)-N(1B)	2.422(4)	N(2B)-Zr(2)-N(1B)	130.78(15)
Zr(2)-P(1B)	2.6777(12)	N(3B)-Zr(2)-P(1B)	103.52(10)
Zr(2)-P(2B)	2.6918(13)	N(2B)-Zr(2)-P(1B)	98.07(11)
		N(1B)-Zr(2)-P(1B)	69.08(8)
		N(3B)-Zr(2)-P(2B)	99.95(11)
		N(2B)-Zr(2)-P(2B)	105.14(11)
		N(1B)-Zr(2)-P(2B)	72.18(8)
		P(1B)-Zr(2)-P(2B)	141.18(4)

Table 4. Bond lengths [Å] and angles [°] for MSW03 (CCDC 787542).

Zr(1)-N(2A)	1.991(4)	P(1B)-C(18B)	1.835(5)
Zr(1)-N(3A)	2.007(3)	P(2B)-C(17B)	1.814(5)
Zr(1)-N(1A)	2.406(3)	P(2B)-C(24B)	1.835(4)
Zr(1)-P(2A)	2.6853(13)	N(1B)-C(7B)	1.350(5)
Zr(1)-P(1A)	2.7002(12)	N(1B)-C(11B)	1.358(5)
P(1A)-C(1A)	1.832(4)	N(2B)-C(31B)	1.446(5)
P(1A)-C(18A)	1.839(5)	N(2B)-C(30B)	1.464(6)
P(2A)-C(17A)	1.836(4)	N(3B)-C(32B)	1.446(5)
P(2A)-C(24A)	1.847(4)	N(3B)-C(33B)	1.457(5)
N(1A)-C(11A)	1.357(5)	C(1B)-C(2B)	1.412(6)
N(1A)-C(7A)	1.358(5)	C(1B)-C(6B)	1.414(6)
N(2A)-C(31A)	1.454(4)	C(2B)-C(3B)	1.384(6)
N(2A)-C(30A)	1.463(5)	C(3B)-C(4B)	1.379(6)
N(3A)-C(33A)	1.466(5)	C(4B)-C(5B)	1.375(6)
N(3A)-C(32A)	1.461(5)	C(5B)-C(6B)	1.392(6)
C(1A)-C(6A)	1.415(6)	C(6B)-C(7B)	1.477(6)
C(1A)-C(2A)	1.433(6)	C(7B)-C(8B)	1.395(6)
C(2A)-C(3A)	1.375(6)	C(8B)-C(9B)	1.364(6)
C(3A)-C(4A)	1.370(6)	C(9B)-C(10B)	1.372(6)
C(4A)-C(5A)	1.376(6)	C(10B)-C(11B)	1.396(6)
C(5A)-C(6A)	1.395(6)	C(11B)-C(12B)	1.484(6)
C(6A)-C(7A)	1.483(6)	C(12B)-C(13B)	1.391(6)
C(7A)-C(8A)	1.385(6)	C(12B)-C(17B)	1.424(6)
C(8A)-C(9A)	1.365(6)	C(13B)-C(14B)	1.374(6)
C(9A)-C(10A)	1.377(6)	C(14B)-C(15B)	1.395(6)
C(10A)-C(11A)	1.391(5)	C(15B)-C(16B)	1.379(6)
C(11A)-C(12A)	1.470(6)	C(16B)-C(17B)	1.393(6)
C(12A)-C(13A)	1.393(6)	C(18B)-C(19B)	1.400(5)
C(12A)-C(17A)	1.426(5)	C(18B)-C(23B)	1.381(6)
C(13A)-C(14A)	1.361(6)	C(19B)-C(20B)	1.382(6)
C(14A)-C(15A)	1.385(5)	C(20B)-C(21B)	1.363(6)
C(15A)-C(16A)	1.367(6)	C(21B)-C(22B)	1.367(6)
C(16A)-C(17A)	1.404(6)	C(22B)-C(23B)	1.387(6)
C(18A)-C(23A)	1.391(5)	C(24B)-C(29B)	1.373(6)
C(18A)-C(19A)	1.411(6)	C(24B)-C(25B)	1.397(6)
C(19A)-C(20A)	1.370(6)	C(25B)-C(26B)	1.369(6)
C(20A)-C(21A)	1.378(6)	C(26B)-C(27B)	1.379(7)
C(21A)-C(22A)	1.373(6)	C(27B)-C(28B)	1.368(6)
C(22A)-C(23A)	1.387(6)	C(28B)-C(29B)	1.389(6)
C(24A)-C(25A)	1.401(6)	C(1C)-C(2C)	1.3900
C(24A)-C(29A)	1.393(6)	C(1C)-C(6C)	1.3900
C(25A)-C(26A)	1.381(5)	C(2C)-C(3C)	1.3900
C(26A)-C(27A)	1.372(6)	C(3C)-C(4C)	1.3900
C(27A)-C(28A)	1.374(6)	C(4C)-C(5C)	1.3900
C(28A)-C(29A)	1.397(5)	C(5C)-C(6C)	1.3900
Zr(2)-N(3B)	1.999(4)		
Zr(2)-N(2B)	2.004(4)	N(2A)-Zr(1)-N(3A)	105.13(14)
Zr(2)-N(1B)	2.422(4)	N(2A)-Zr(1)-N(1A)	119.45(14)
Zr(2)-P(1B)	2.6777(12)	N(3A)-Zr(1)-N(1A)	135.20(14)
Zr(2)-P(2B)	2.6918(13)	N(2A)-Zr(1)-P(2A)	105.13(10)
P(1B)-C(1B)	1.831(5)	N(3A)-Zr(1)-P(2A)	96.56(10)

N(1A)-Zr(1)-P(2A)	69.05(8)	C(22A)-C(21A)-C(20A)	119.4(5)
N(2A)-Zr(1)-P(1A)	101.19(10)	C(21A)-C(22A)-C(23A)	121.1(5)
N(3A)-Zr(1)-P(1A)	103.47(10)	C(18A)-C(23A)-C(22A)	120.8(4)
N(1A)-Zr(1)-P(1A)	73.39(9)	C(25A)-C(24A)-C(29A)	118.2(4)
P(2A)-Zr(1)-P(1A)	141.26(4)	C(25A)-C(24A)-P(2A)	118.7(3)
C(1A)-P(1A)-C(18A)	102.7(2)	C(29A)-C(24A)-P(2A)	122.7(3)
C(1A)-P(1A)-Zr(1)	80.20(13)	C(26A)-C(25A)-C(24A)	120.6(4)
C(18A)-P(1A)-Zr(1)	109.76(14)	C(27A)-C(26A)-C(25A)	120.4(4)
C(17A)-P(2A)-C(24A)	102.18(19)	C(26A)-C(27A)-C(28A)	120.4(4)
C(17A)-P(2A)-Zr(1)	83.56(14)	C(27A)-C(28A)-C(29A)	119.8(4)
C(24A)-P(2A)-Zr(1)	115.08(15)	C(24A)-C(29A)-C(28A)	120.6(4)
C(11A)-N(1A)-C(7A)	119.2(4)	N(3B)-Zr(2)-N(2B)	105.09(16)
C(11A)-N(1A)-Zr(1)	121.4(3)	N(3B)-Zr(2)-N(1B)	123.98(15)
C(7A)-N(1A)-Zr(1)	119.4(3)	N(2B)-Zr(2)-N(1B)	130.78(15)
C(31A)-N(2A)-C(30A)	110.4(3)	N(3B)-Zr(2)-P(1B)	103.52(10)
C(31A)-N(2A)-Zr(1)	130.4(3)	N(2B)-Zr(2)-P(1B)	98.07(11)
C(30A)-N(2A)-Zr(1)	117.6(3)	N(1B)-Zr(2)-P(1B)	69.08(8)
C(33A)-N(3A)-C(32A)	110.6(3)	N(3B)-Zr(2)-P(2B)	99.95(11)
C(33A)-N(3A)-Zr(1)	126.1(3)	N(2B)-Zr(2)-P(2B)	105.14(11)
C(32A)-N(3A)-Zr(1)	123.3(3)	N(1B)-Zr(2)-P(2B)	72.18(8)
C(6A)-C(1A)-C(2A)	116.5(4)	P(1B)-Zr(2)-P(2B)	141.18(4)
C(6A)-C(1A)-P(1A)	119.6(4)	C(1B)-P(1B)-C(18B)	104.2(2)
C(2A)-C(1A)-P(1A)	123.9(4)	C(1B)-P(1B)-Zr(2)	88.81(13)
C(3A)-C(2A)-C(1A)	121.3(5)	C(18B)-P(1B)-Zr(2)	113.21(15)
C(4A)-C(3A)-C(2A)	121.2(5)	C(17B)-P(2B)-C(24B)	102.4(2)
C(3A)-C(4A)-C(5A)	119.1(5)	C(17B)-P(2B)-Zr(2)	80.42(15)
C(4A)-C(5A)-C(6A)	122.0(5)	C(24B)-P(2B)-Zr(2)	107.96(16)
C(5A)-C(6A)-C(1A)	119.9(4)	C(7B)-N(1B)-C(11B)	119.2(4)
C(5A)-C(6A)-C(7A)	118.2(4)	C(7B)-N(1B)-Zr(2)	123.6(3)
C(1A)-C(6A)-C(7A)	121.9(4)	C(11B)-N(1B)-Zr(2)	117.1(3)
N(1A)-C(7A)-C(8A)	121.0(5)	C(31B)-N(2B)-C(30B)	110.0(4)
N(1A)-C(7A)-C(6A)	117.4(4)	C(31B)-N(2B)-Zr(2)	132.6(3)
C(8A)-C(7A)-C(6A)	121.5(4)	C(30B)-N(2B)-Zr(2)	116.9(3)
C(9A)-C(8A)-C(7A)	119.8(5)	C(32B)-N(3B)-C(33B)	111.7(4)
C(8A)-C(9A)-C(10A)	119.7(5)	C(32B)-N(3B)-Zr(2)	111.6(3)
C(11A)-C(10A)-C(9A)	119.3(5)	C(33B)-N(3B)-Zr(2)	136.7(4)
N(1A)-C(11A)-C(10A)	120.9(4)	C(2B)-C(1B)-C(6B)	116.0(4)
N(1A)-C(11A)-C(12A)	118.3(4)	C(2B)-C(1B)-P(1B)	123.5(4)
C(10A)-C(11A)-C(12A)	120.7(4)	C(6B)-C(1B)-P(1B)	120.4(4)
C(13A)-C(12A)-C(17A)	119.3(4)	C(3B)-C(2B)-C(1B)	122.4(5)
C(13A)-C(12A)-C(11A)	120.2(4)	C(4B)-C(3B)-C(2B)	120.4(5)
C(17A)-C(12A)-C(11A)	120.4(4)	C(5B)-C(4B)-C(3B)	118.6(5)
C(14A)-C(13A)-C(12A)	123.2(4)	C(4B)-C(5B)-C(6B)	122.1(5)
C(13A)-C(14A)-C(15A)	117.9(5)	C(5B)-C(6B)-C(1B)	120.4(4)
C(16A)-C(15A)-C(14A)	120.6(4)	C(5B)-C(6B)-C(7B)	119.6(4)
C(15A)-C(16A)-C(17A)	123.0(4)	C(1B)-C(6B)-C(7B)	119.9(4)
C(16A)-C(17A)-C(12A)	115.8(4)	N(1B)-C(7B)-C(8B)	120.6(4)
C(16A)-C(17A)-P(2A)	124.2(3)	N(1B)-C(7B)-C(6B)	119.6(4)
C(12A)-C(17A)-P(2A)	120.0(3)	C(8B)-C(7B)-C(6B)	119.7(4)
C(23A)-C(18A)-C(19A)	116.7(4)	C(9B)-C(8B)-C(7B)	120.4(5)
C(23A)-C(18A)-P(1A)	122.2(4)	C(8B)-C(9B)-C(10B)	119.1(5)
C(19A)-C(18A)-P(1A)	120.9(4)	C(9B)-C(10B)-C(11B)	119.5(5)
C(20A)-C(19A)-C(18A)	122.1(4)	N(1B)-C(11B)-C(10B)	121.0(4)
C(21A)-C(20A)-C(19A)	119.9(5)	N(1B)-C(11B)-C(12B)	118.7(4)

C(10B)-C(11B)-C(12B)	120.2(5)	C(21B)-C(22B)-C(23B)	121.1(5)
C(13B)-C(12B)-C(17B)	120.8(5)	C(22B)-C(23B)-C(18B)	121.0(4)
C(13B)-C(12B)-C(11B)	117.7(4)	C(29B)-C(24B)-C(25B)	117.5(4)
C(17B)-C(12B)-C(11B)	121.5(4)	C(29B)-C(24B)-P(2B)	122.0(4)
C(14B)-C(13B)-C(12B)	121.3(5)	C(25B)-C(24B)-P(2B)	120.3(4)
C(13B)-C(14B)-C(15B)	119.1(5)	C(26B)-C(25B)-C(24B)	120.7(5)
C(16B)-C(15B)-C(14B)	119.6(5)	C(27B)-C(26B)-C(25B)	121.2(5)
C(15B)-C(16B)-C(17B)	123.3(5)	C(26B)-C(27B)-C(28B)	118.8(5)
C(16B)-C(17B)-C(12B)	115.9(4)	C(27B)-C(28B)-C(29B)	120.1(5)
C(16B)-C(17B)-P(2B)	124.3(4)	C(24B)-C(29B)-C(28B)	121.7(4)
C(12B)-C(17B)-P(2B)	119.8(4)	C(2C)-C(1C)-C(6C)	120.0
C(19B)-C(18B)-C(23B)	116.9(4)	C(3C)-C(2C)-C(1C)	120.0
C(19B)-C(18B)-P(1B)	118.2(4)	C(2C)-C(3C)-C(4C)	120.0
C(23B)-C(18B)-P(1B)	124.4(3)	C(5C)-C(4C)-C(3C)	120.0
C(20B)-C(19B)-C(18B)	121.6(4)	C(6C)-C(5C)-C(4C)	120.0
C(19B)-C(20B)-C(21B)	120.3(4)	C(5C)-C(6C)-C(1C)	120.0
C(22B)-C(21B)-C(20B)	119.2(5)		

Table 5. Anisotropic displacement parameters ($Å^2 x 10^4$) for MSW03 (CCDC 787542). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Zr(1)	160(3)	147(3)	157(3)	-7(2)	8(2)	-8(2)
P(1A)	162(7)	173(8)	202(8)	9(6)	20(6)	-13(6)
P(2A)	169(8)	172(8)	167(8)	-2(6)	-4(6)	-12(6)
N(1A)	130(20)	200(30)	150(20)	0(20)	-27(18)	0(20)
N(2A)	210(20)	190(30)	170(20)	14(19)	16(18)	-30(20)
N(3A)	230(20)	190(30)	130(20)	-31(19)	6(18)	-20(20)
C(1A)	170(30)	230(30)	110(30)	50(20)	40(20)	-10(30)
C(2A)	190(30)	260(30)	190(30)	30(20)	-20(20)	30(30)
C(3A)	220(30)	270(40)	250(30)	100(30)	-10(20)	-130(30)
C(4A)	210(30)	370(40)	320(30)	90(30)	120(20)	-10(30)
C(5A)	250(30)	270(40)	220(30)	30(30)	80(20)	100(30)
C(6A)	170(30)	190(30)	120(30)	40(20)	20(20)	20(30)
C(7A)	130(30)	280(30)	160(30)	10(30)	0(20)	90(20)
C(8A)	270(30)	250(30)	150(30)	-50(30)	40(20)	40(30)
C(9A)	260(30)	310(40)	230(30)	-100(30)	-30(20)	80(30)
C(10A)	180(30)	160(30)	280(30)	-40(30)	-50(20)	30(20)
C(11A)	90(30)	160(30)	180(30)	-10(30)	-30(20)	30(20)
C(12A)	170(30)	100(30)	190(30)	-50(20)	0(20)	30(20)
C(13A)	140(30)	170(30)	300(30)	-30(30)	-40(20)	30(30)
C(14A)	170(30)	180(30)	420(40)	30(30)	20(30)	-60(20)
C(15A)	270(30)	220(30)	270(30)	80(30)	70(20)	-40(30)
C(16A)	160(30)	230(30)	240(30)	-20(30)	-20(20)	0(30)
C(17A)	150(30)	100(30)	200(30)	20(20)	10(20)	10(20)
C(18A)	110(30)	140(30)	250(30)	0(30)	10(20)	-20(20)
C(19A)	240(30)	280(30)	150(30)	20(30)	-10(20)	-10(30)
C(20A)	290(30)	150(30)	360(40)	30(30)	-50(30)	50(30)
C(21A)	270(30)	150(30)	420(40)	-10(30)	20(30)	50(30)
C(22A)	270(30)	340(40)	280(30)	-60(30)	80(20)	0(30)
C(23A)	210(30)	170(30)	290(30)	0(30)	70(20)	-10(30)
C(24A)	110(30)	200(30)	170(30)	10(20)	30(20)	-40(20)
C(25A)	240(30)	180(30)	240(30)	0(20)	30(20)	-30(30)
C(26A)	250(30)	220(30)	240(30)	80(30)	-60(20)	0(30)
C(27A)	240(30)	330(40)	150(30)	80(30)	-80(20)	-40(30)
C(28A)	270(30)	310(40)	190(30)	-50(30)	-50(20)	-10(30)
C(29A)	230(30)	210(30)	210(30)	40(30)	20(20)	40(20)
C(30A)	310(30)	370(40)	290(30)	60(30)	50(30)	-120(30)
C(31A)	370(30)	310(40)	260(30)	-30(30)	70(20)	-20(30)
C(32A)	270(30)	270(30)	260(30)	20(30)	-40(20)	-50(30)
C(33A)	360(30)	230(30)	280(30)	20(30)	-40(30)	-60(30)
Zr(2)	202(3)	169(3)	196(3)	-7(2)	24(2)	4(3)
P(1B)	192(8)	161(8)	252(8)	-9(6)	19(6)	5(6)
P(2B)	208(8)	254(9)	213(8)	-9(7)	32(6)	31(7)
N(1B)	200(20)	130(30)	220(30)	40(20)	-29(19)	20(20)
N(2B)	310(30)	280(30)	210(30)	0(20)	50(20)	90(20)
N(3B)	260(30)	230(30)	200(30)	20(20)	-11(19)	-50(20)
C(1B)	180(30)	160(30)	190(30)	-60(20)	-40(20)	-10(20)

C(2B)	270(30)	130(30)	230(30)	-30(30)	0(20)	40(30)
C(3B)	290(30)	280(40)	250(30)	0(30)	60(30)	-30(30)
C(4B)	280(30)	390(40)	170(30)	-30(30)	60(20)	-20(30)
C(5B)	220(30)	200(30)	220(30)	-80(30)	-30(20)	50(30)
C(6B)	140(30)	160(30)	130(30)	-30(20)	-50(20)	-20(20)
C(7B)	120(30)	220(30)	190(30)	-50(30)	-70(20)	90(20)
C(8B)	260(30)	180(30)	230(30)	-20(30)	-90(20)	120(30)
C(9B)	290(30)	170(30)	360(40)	-70(30)	-160(30)	90(30)
C(10B)	230(30)	150(30)	440(40)	50(30)	-40(30)	0(30)
C(11B)	130(30)	220(30)	280(30)	-10(30)	-30(20)	40(30)
C(12B)	280(30)	140(30)	280(30)	60(30)	90(30)	40(30)
C(13B)	380(40)	350(40)	390(40)	140(30)	60(30)	-70(30)
C(14B)	380(40)	540(50)	580(40)	220(40)	180(30)	-160(30)
C(15B)	550(40)	490(40)	340(40)	120(30)	160(30)	-80(40)
C(16B)	300(40)	320(40)	330(40)	70(30)	40(30)	-30(30)
C(17B)	310(30)	200(30)	190(30)	50(30)	70(30)	20(30)
C(18B)	200(30)	180(30)	210(30)	0(20)	70(20)	0(20)
C(19B)	320(30)	220(30)	190(30)	-20(20)	30(20)	70(30)
C(20B)	320(30)	270(40)	240(30)	60(30)	-10(20)	90(30)
C(21B)	310(30)	210(30)	360(30)	0(30)	10(30)	110(30)
C(22B)	490(40)	220(40)	600(40)	-150(30)	-220(30)	90(30)
C(23B)	330(30)	150(30)	520(40)	-60(30)	-170(30)	70(30)
C(24B)	190(30)	250(30)	190(30)	-30(30)	50(20)	10(30)
C(25B)	490(40)	270(40)	300(30)	-10(30)	-40(30)	110(30)
C(26B)	710(50)	450(50)	270(40)	30(30)	-110(30)	140(40)
C(27B)	480(40)	570(50)	190(30)	-150(30)	-40(30)	40(40)
C(28B)	430(40)	340(40)	260(30)	-10(30)	60(30)	-50(30)
C(29B)	300(30)	370(40)	180(30)	0(30)	20(20)	-10(30)
C(30B)	420(40)	590(40)	380(40)	110(30)	180(30)	160(40)
C(31B)	670(40)	510(40)	360(40)	-140(30)	50(30)	200(40)
C(32B)	280(30)	610(40)	290(40)	70(30)	-10(30)	-150(30)
C(33B)	510(40)	270(40)	540(40)	70(30)	-110(30)	-110(30)